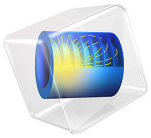


Model created in COMSOL Multiphysics 6.4

Lithium-Sulfur Battery

Introduction

Lithium-sulfur (Li-S) batteries are used in niche applications with high demands for specific energy densities, which may be as high as 500–600 Wh/kg.

The chemistry is complex, with multiple polysulfide species participating in several charge transfer reactions. The chemistry also involves precipitation and dissolution of multiple solid species.

This example models discharge of a Li-S cell at two different discharge rates. The electrolyte charge and mass transport of a lithium salt and 6 polysulfides is included, as well as the precipitation-dissolution of solid octasulfur (S_8) and lithium sulfide (Li_2S) in the separator and positive electrode.

The model is based on a paper by Zhang and others (Ref. 1).

Model Definition

The 1D model geometry is shown in Figure 1. The separator and the positive (cathode during discharge) porous electrode are defined as domains in the geometry. The leftmost

boundary represents the negative lithium metal electrode, and the rightmost boundary represents the positive metal current collector.

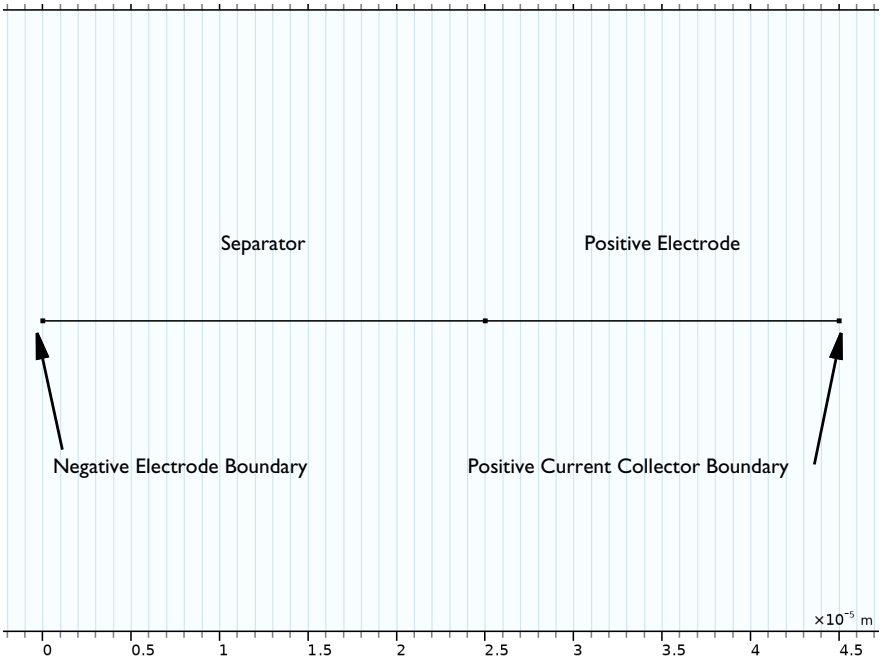


Figure 1: Model geometry.

The electrolyte mass and charge transport are modeled using the Nernst-Planck equations with electroneutrality.

The following five charge transfer reactions and six participating polysulfide species are considered in the positive electrode domain:

$$\frac{1}{2}S_8 + e^- \Leftrightarrow \frac{1}{2}S_8^{2-} \tag{1}$$

$$\frac{3}{2}S_8^{2-} + e^- \Leftrightarrow 2S_6^{2-} \tag{2}$$

$$S_6^{2-} + e^- \Leftrightarrow \frac{3}{2}S_4^{2-} \tag{3}$$

$$\frac{1}{2}S_4^{2-} + e^- \Leftrightarrow S_2^{2-} \tag{4}$$

$$\frac{1}{2}S_2^{2-} + e^- \Leftrightarrow S^{2-} \tag{5}$$

The charge transfer reactions are defined using the Nernst equation in combination with the Butler–Volmer equation, assuming the law of mass action.

In addition to the above six polysulfide species, also the species Li^+ and A^- are included in the electrolyte, where A^- is the counter anion of the lithium salt. The same species are also present in the separator domain.

Two precipitation-dissolution (nonfaradaic) reactions involving the solid species S_8 and Li_2S are included in the model (in both the domains) according to

$$S_8(s) \Leftrightarrow S_8 \tag{6}$$

$$2Li^+ + S^{2-} \Leftrightarrow Li_2S(s) \tag{7}$$

The model is solved for two different discharge rates: 0.2C and 1C.

Results and Discussion

Figure 1 shows the cell voltages during a 0.2C and a 1C discharge. The voltage and capacity gets significantly lowered for the higher discharge rate.

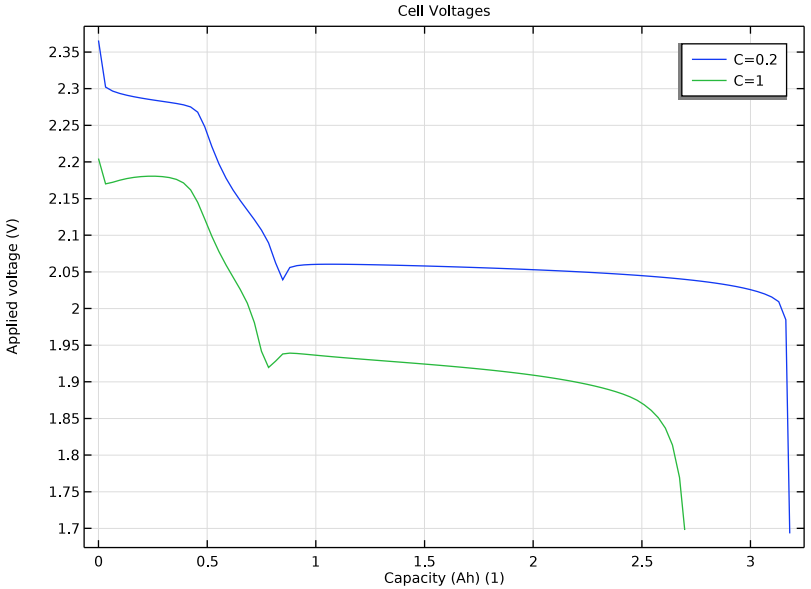


Figure 2: Voltage discharge curves at 0.2C and 1C.

Figure 3 and Figure 4 show the concentration profiles in the cell at end of discharge at 0.2C and 1C, respectively. The amount of remaining polysulfide species correspond to the lowered capacity at 1C compared 0.2C that was seen in Figure 2.

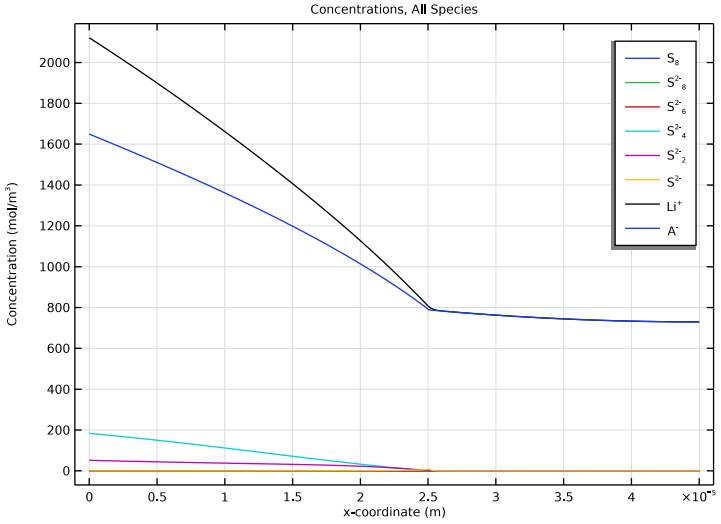


Figure 3: Concentration of electrolyte species at end of discharge at 0.2C.

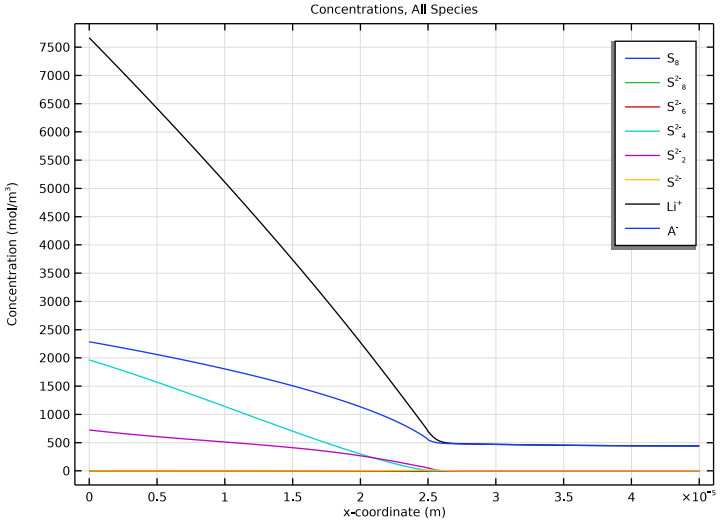


Figure 4: Concentration of electrolyte species at end of discharge at 1C.

Finally, Figure 5 and Figure 6 show the volume fraction profiles of $Li_2S(s)$ during discharge at 0.2C and 1C, respectively. The 1C profiles are generally less uniform than the profiles at 0.2C, indicating a less uniform current distribution for the higher discharge rate.

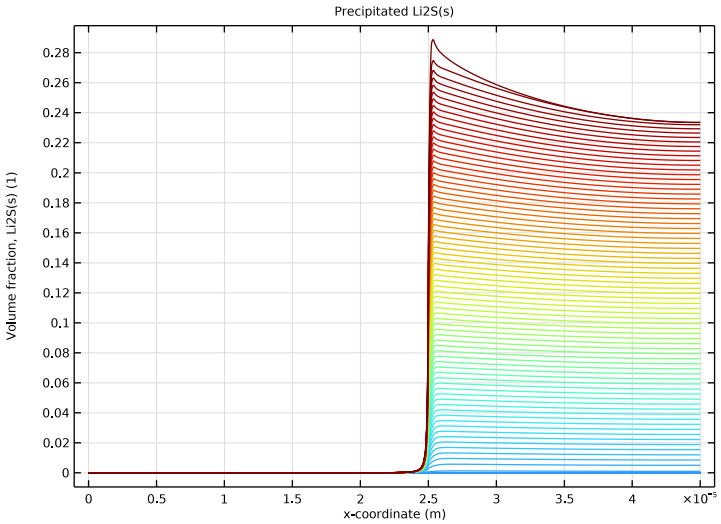


Figure 5: Volume fraction profiles of $Li_2S(s)$ during discharge at 0.2C.

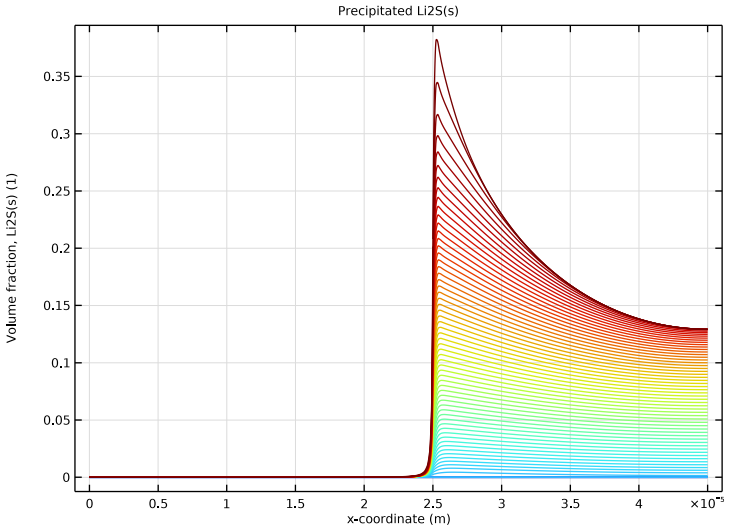


Figure 6: Volume fraction profiles of $Li_2S(s)$ during discharge at 1C.

Reference

1. T. Zhang, M. Marinescu, S. Walus, and G. Offer, "Modeling transport-limited discharge capacity of lithium-sulfur cells," *Electrochimica Acta*, vol. 219, pp. 502–508, 2016.

Application Library path: `Battery_Design_Module/Batteries,_General/lithium_sulfur`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click — **1D**.

2 In the **Select Physics** tree, select **Electrochemistry** > **Tertiary Current Distribution, Nernst–Planck** > **Tertiary, Electroneutrality (tcd)**.

3 Click **Add**.

4 In the **Number of species** text field, type `8`.

Type in the names of the electrolyte concentration variables in the table as follows. (The solid S8(s) and Li2S(s) species will be added later.)

5 In the **Concentrations (mol/m³)** table, enter the following settings:

`S8`
`S8_2m`
`S6_2m`
`S4_2m`
`S2_2m`
`S_2m`
`Li_1p`
`A_1m`

6 Click **Study**.

7 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Initialization**.

8 Click **Done**.

TERTIARY CURRENT DISTRIBUTION, NERNST–PLANCK (TCD)

The Nernst-Planck model assumes electroneutrality, and eliminates one of the concentration-dependent variables based on the electroneutrality condition. For this model it is suitable to select the `A_1m` (the electrolyte salt anion) as to be taken from electroneutrality since its concentration is relatively high in relation to the other species, and since it does not participate in any electrode reactions.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst–Planck (tcd)**.

2 In the **Settings** window for **Tertiary Current Distribution, Nernst–Planck**, locate the **Electrolyte Charge Conservation** section.

3 From the **From electroneutrality** list, choose **A_1m**.

GLOBAL DEFINITIONS

Parameters 1

Load the model parameters from a text file.

1. In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `lithium_sulfur_parameters.txt`.

GEOMETRY 1

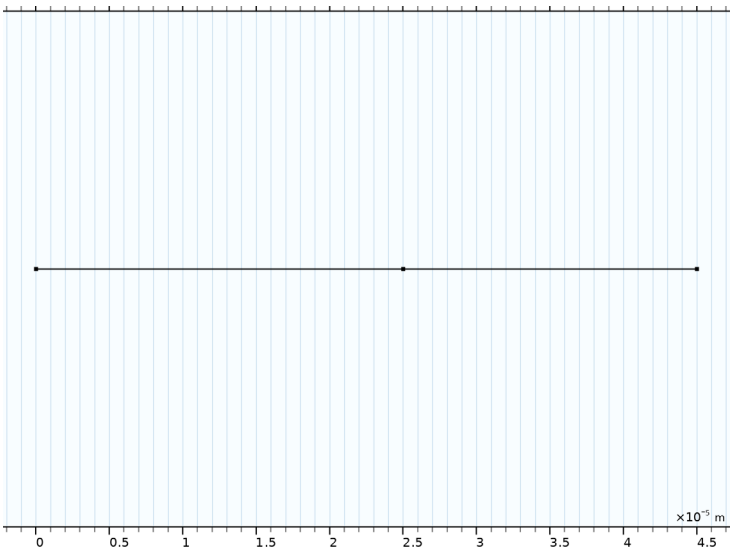
Interval 1 (i1)

The geometry consists of two domains: the positive porous electrode and the separator. The negative electrode is modeled as a boundary condition and is not added as a domain at this point.

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.
2. In the **Settings** window for **Interval**, locate the **Interval** section.
3. From the **Specify** list, choose **Interval lengths**.
4. In the table, enter the following settings:

Lengths (m)
L_sep
L_pos

5 Click **Build Selected**.



TERTIARY CURRENT DISTRIBUTION, NERNST–PLANCK (TCD)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst–Planck (tcd)**.

2 In the **Settings** window for **Tertiary Current Distribution, Nernst–Planck**, locate the **Cross-Sectional Area** section.

3 In the A_c text field, type `A_cell`.

Start setting up the physics for charge and mass transport in the separator.

Species Charges 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Species Charges 1**.

2 In the **Settings** window for **Species Charges**, locate the **Charge** section.

3 In the z_{S82m} text field, type `-2`.

4 In the z_{S62m} text field, type `-2`.

5 In the z_{S42m} text field, type `-2`.

6 In the z_{S22m} text field, type `-2`.

7 In the z_{S2m} text field, type `-2`.

8 In the z_{Li1p} text field, type `1`.

9 In the z_{A1m} text field, type `-1`.

Separator 1

1 In the **Physics** toolbar, click **Domains** and choose **Separator**.

2 Select Domain 1 only.

3 In the **Settings** window for **Separator**, locate the **Diffusion** section.

4 In the D_{S8} text field, type `D_S8`.

5 In the D_{S82m} text field, type `D_S8_2m`.

6 In the D_{S62m} text field, type `D_S6_2m`.

7 In the D_{S42m} text field, type `D_S4_2m`.

8 In the D_{S22m} text field, type `D_S2_2m`.

9 In the D_{S2m} text field, type `D_S_2m`.

10 In the D_{Li1p} text field, type `D_Li_1p`.

11 In the D_{A1m} text field, type `D_A_1m`.

12 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_sep_0`.

Note that, by default, the diffusion coefficients will be corrected by a Bruggeman relation to account for the effect of the pore network.

Porous Electrode 1

Add similar settings for the positive electrode.

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode**.

2 Select Domain 2 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Diffusion** section.

4 In the D_{S8} text field, type `D_S8`.

5 In the D_{S82m} text field, type `D_S8_2m`.

6 In the D_{S62m} text field, type `D_S6_2m`.

7 In the D_{S42m} text field, type `D_S4_2m`.

8 In the D_{S22m} text field, type `D_S2_2m`.

9 In the D_{S2m} text field, type `D_S_2m`.

10 In the D_{Li1p} text field, type `D_Li_1p`.

11 In the D_{A1m} text field, type `D_A_1m`.

12 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type `sigma_s`.

13 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `1-epsl_pos_0`.

14 In the ε_l text field, type `epsl_pos_0`.

For the electrode phase assume that the conductivity value entered is the effective conductivity and hence already accounts for the porous structure:

15 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.

Porous Electrode Reaction 1

Now start setting up the electrode kinetics. In total, there are five active electrode reactions in the porous electrode.

1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{S8} text field, type `-1/2`.

4 In the ν_{S82m} text field, type `1/2`.

5 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_1_ref`.

6 Click to expand the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
S8	`c_S8_ref`
S8_2m	`c_S8_2m_ref`

7 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_1_ref`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_pos`.

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Porous Electrode Reaction 2

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Electrode Reaction**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{S82m} text field, type `-3/2`.

4 In the ν_{S62m} text field, type `2`.

5 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_2_ref`.

6 Locate the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
S8_2m	c_S8_2m_ref
S6_2m	c_S6_2m_ref

7 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_2_ref`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_pos`.

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Porous Electrode Reaction 3

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Electrode Reaction**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{S62m} text field, type `-1`.

4 In the ν_{S42m} text field, type `3/2`.

5 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_3_ref`.

6 Locate the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
S6_2m	c_S6_2m_ref
S4_2m	c_S4_2m_ref

7 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_3_ref`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_pos`.

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Porous Electrode Reaction 4

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Electrode Reaction**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{S42m} text field, type `-1/2`.

4 In the ν_{S22m} text field, type `1`.

5 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_4_ref`.

6 Locate the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
S4_2m	c_S4_2m_ref
S2_2m	c_S2_2m_ref

7 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_4_ref`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_pos`.

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Porous Electrode Reaction 5

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Electrode Reaction**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{S22m} text field, type `-1/2`.

4 In the ν_{S2m} text field, type `1`.

5 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_5_ref`.

6 Locate the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
S2_2m	c_S2_2m_ref
S_2m	c_S_2m_ref

7 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_5_ref`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av_pos`.

Separator 1

There are also two solid species in the model. Define these in the separator as follows:

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Separator 1**.

2 In the **Settings** window for **Separator**, click to expand the **Dissolving–Depositing Species** section.

3 Click **Add**.

4 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Li2S_s	rho_Li2S_s	M_Li2S_s

Add the settings for S8(s) in a second row in the table as follows:

5 Click + **Add**.

6 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
S8_s	rho_S8_s	M_S8_s

Porous Electrode 1

The same solid species are also present in the electrode.

1 In the **Model Builder** window, click **Porous Electrode 1**.

2 In the **Settings** window for **Porous Electrode**, click to expand the **Dissolving–Depositing Species** section.

3 Click + **Add**.

4 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Li2S_s	rho_Li2S_s	M_Li2S_s

Also for the porous electrode, add the settings for S8(s) in a second row in the table:

5 Click + **Add**.

6 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
S8_s	rho_S8_s	M_S8_s

DEFINITIONS

Now define the dissolution-precipitation rates of the solid species.

Variables - Separator

Import some variable expressions for the separator that define the volume fractions of the solid species. These expressions are based on the automatically defined concentration variables for each species set up in the **Depositing-Dissolving Species** section of the separator node.

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - Separator` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `lithium_sulfur_separator_variables.txt`.

Variables - Positive Electrode

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - Positive Electrode` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 2 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `lithium_sulfur_electrode_variables.txt`.

Note that an expression for the specific surface area, which depends on the local electrolyte volume fraction, is also present in the variables you just imported.

Variables - All Domains

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - All Domains` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `lithium_sulfur_all_domains_variables.txt`.

The next step is to add these rate expressions as **Nonfaradaic Reactions** in each domain, together with initial values for the solid concentration variables.

Non-Faradaic Reactions - Li2S(s)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** > **Separator 1** click **Nonfaradaic Reactions 1**.

2 In the **Settings** window for **Nonfaradaic Reactions**, type `Non-Faradaic Reactions - Li2S(s)` in the **Label** text field.

Use the `R_Li2S_s` rate variable to set the rate for `S_2m`, `Li_1p`, and `Li2S_s` as follows:

3 Locate the **Reaction Rate** section. In the R_{S2m} text field, type `-R_Li2S_s/tcd.epsl`.

4 In the R_{Li1p} text field, type `-2*R_Li2S_s/tcd.epsl`.

5 In the **Reaction rate for dissolving–depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
Li2S_s	R_Li2S_s

Separator 1

In the **Model Builder** window, click **Separator 1**.

Non-Faradaic Reactions - S8(s)

1 In the **Physics** toolbar, click **Attributes** and choose **Nonfaradaic Reactions**.

2 In the **Settings** window for **Nonfaradaic Reactions**, type `Non-Faradaic Reactions - S8(s)` in the **Label** text field.

Here, use the `R_S8_s` rate variable to set the rate for `S8` and `S8_s`:

3 Locate the **Reaction Rate** section. In the R_{S8} text field, type `-R_S8_s/tcd.epsl`.

4 In the **Reaction rate for dissolving–depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
S8_s	R_S8_s

Separator 1

In the **Model Builder** window, click **Separator 1**.

Initial Values for Dissolving–Depositing Species 1

1 In the **Physics** toolbar, click **Attributes** and choose **Initial Values for Dissolving–Depositing Species**.

2 In the **Settings** window for **Initial Values for Dissolving–Depositing Species**, locate the **Initial Values for Dissolving–Depositing Species** section.

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
Li2S_s	eps_Li2S_s_sep_0/Vm_Li2S_s
S8_s	eps_S8_s_sep_0/Vm_S8_s

Porous Electrode 1

In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Porous Electrode 1**.

Non-Faradaic Reactions - Li2S(s)

1 In the **Physics** toolbar, click **Attributes** and choose **Nonfaradaic Reactions**.

2 In the **Settings** window for **Nonfaradaic Reactions**, type `Non-Faradaic Reactions - Li2S(s)` in the **Label** text field.

3 Locate the **Reaction Rate** section. In the R_{S2m} text field, type `-R_Li2S_s/tcd.epsl`.

4 In the R_{Li1p} text field, type `-2*R_Li2S_s/tcd.epsl`.

5 In the **Reaction rate for dissolving–depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
Li2S_s	R_Li2S_s

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Non-Faradaic Reactions - S8(s)

1 In the **Physics** toolbar, click **Attributes** and choose **Nonfaradaic Reactions**.

2 In the **Settings** window for **Nonfaradaic Reactions**, type `Non-Faradaic Reactions - S8(s)` in the **Label** text field.

3 Locate the **Reaction Rate** section. In the R_{S8} text field, type `-R_S8_s/tcd.epsl`.

4 In the **Reaction rate for dissolving–depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
S8_s	R_S8_s

Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Initial Values for Dissolving–Depositing Species 1

1 In the **Physics** toolbar, click **Attributes** and choose **Initial Values for Dissolving–Depositing Species**.

2 In the **Settings** window for **Initial Values for Dissolving–Depositing Species**, locate the **Initial Values for Dissolving–Depositing Species** section.

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
Li2S_s	eps_Li2S_s_pos_0/Vm_Li2S_s
S8_s	eps_S8_s_pos_0/Vm_S8_s

Electrode Surface 1

Specify the negative electrode and electrode reaction (Li/Li+) as follows:

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface**.

2 Select Boundary 1 only.

This boundary is to be grounded, so the default voltage setting of 0 V does not need to be changed.

Electrode Reaction 1

1 In the **Model Builder** window, click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{Li1p} text field, type `-1`.

4 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_Li_ref`.

5 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_Li_ref`.

Load Cycle 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Load Cycle**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Load Cycle**, locate the **Load Type** section.

4 From the list, choose **Galvanostatic**.

5 Locate the **Cycling Stop Condition** section. From the list, choose **Minimum voltage**.

6 In the E_{min} text field, type `1.7[V]`.

7 Locate the **Probes** section. Select the **Applied voltage** checkbox.

The probe will plot the cell voltage while solving.

DEFINITIONS

Load Cycle Probe (tcd_lc1_volt)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions** click **Load Cycle Probe (tcd_lc1_volt)**.

2 In the **Settings** window for **Global Variable Probe**, locate the **Expression** section.

3 Select the **Description** checkbox. In the associated text field, type `Cell voltage`.

TERTIARY CURRENT DISTRIBUTION, NERNST–PLANCK (TCD)

Load Cycle 1

In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Load Cycle 1**.

Current 1

1 In the **Physics** toolbar, click **Attributes** and choose **Current**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Current**, locate the **Current** section.

4 In the I_{set} text field, type `-I_1C*C`.

You will vary the parameter `C` later when solving the model to simulate different discharge rates.

Initial Values 1

Now set the initial concentrations for the electrolyte species.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst–Planck (tcd)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $S8$ text field, type `c_S8_ref`.

4 In the $S8_{2\text{m}}$ text field, type `c_S8_2m_ref`.

5 In the $S6_{2\text{m}}$ text field, type `c_S6_2m_ref`.

6 In the $S4_{2\text{m}}$ text field, type `c_S4_2m_ref`.

7 In the $S2_{2\text{m}}$ text field, type `c_S2_2m_ref`.

8 In the $S_{2\text{m}}$ text field, type `c_S_2m_ref`.

9 In the $Li_{1\text{p}}$ text field, type `c_Li_1p_ref`.

10 In the *phis* text field, type `Eeq_1_ref`.

MESH 1

All the necessary physics settings are now completed. Due to steep gradients of the Li2S(s) species, this model needs a very well resolved mesh close to the separator-positive electrode boundary. Modify the default mesh as follows:

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 1

1 In the **Model Builder** window, right-click **Edge 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 2 only.

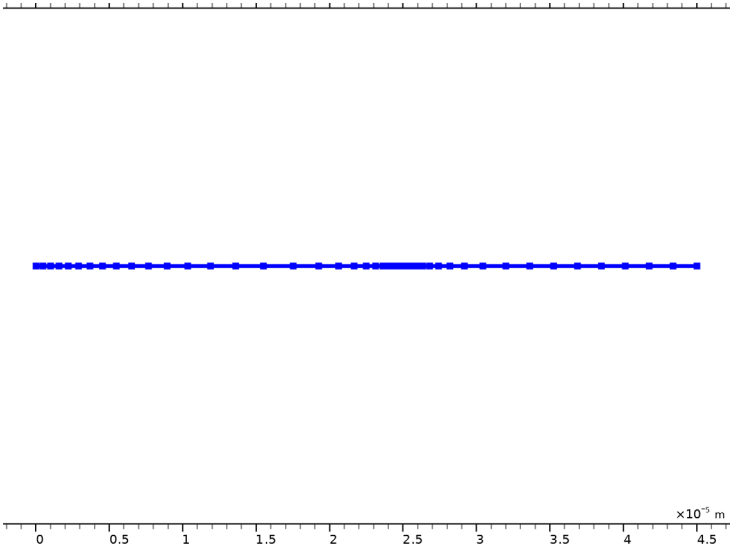
5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

7 Select the **Maximum element size** checkbox. In the associated text field, type `1e-7`.

Edge 1

Right-click **Edge 1** and choose **Build All**.



STUDY 1

Next, set up the solver sequence. Add a parametric sweep to solve for a range of different C-rates.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C (C-rate)	`0.2 1`	

The above settings mean that the study will solve for two different current-density boundary conditions as defined in the **Electrode Current Density** node you added before.

Step 2: Time Dependent

Now set the times of the time-dependent solver. Use the `C`-parameter to solve for a range of time steps corresponding to a range from 100% to (minimum) 0% nominal state of charge.

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 From the **Time unit** list, choose **h**.

4 In the **Output times** text field, type `range(0,0.01/C,1/C)`.

The model is now ready for solving. It will take about a minute to solve.

5 In the **Study** toolbar, click **Compute**.

Modify the first default plot to show the cell voltage versus capacity.

RESULTS

Cell Voltages

1 In the **Model Builder** window, under **Results** click **Boundary Electrode Potential with Respect to Ground (tcd)**.

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltages` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Cell Voltages** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `t*C*I_1C/1[A*h]`.

5 Select the **Description** checkbox. In the associated text field, type `Capacity (Ah)`.

6 Click to expand the **Legends** section. Select the **Show legends** checkbox.

7 Find the **Include** subsection. Clear the **Description** checkbox.

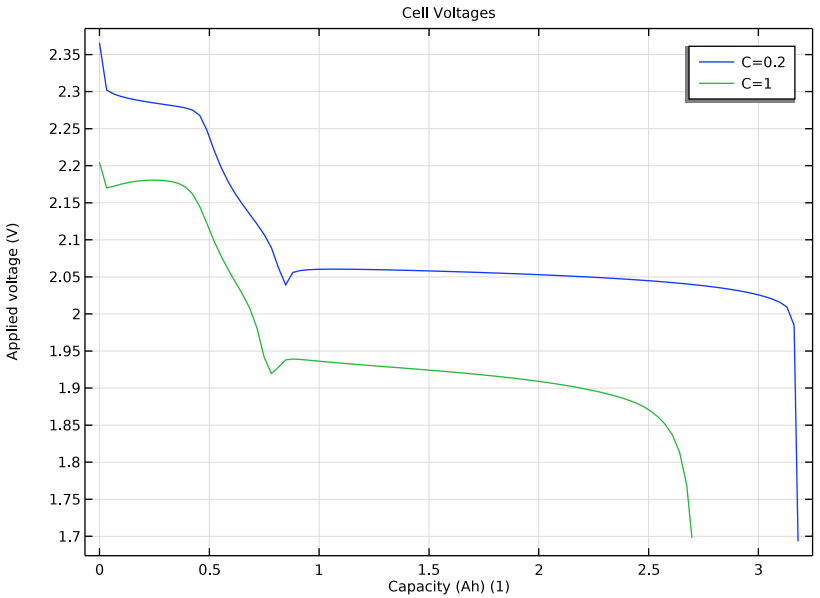
Cell Voltages

1 In the **Model Builder** window, click **Cell Voltages**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Label**.

4 In the **Cell Voltages** toolbar, click **Plot**.



Concentrations, All Species (tcd)

Now modify the default concentration plot to show only the last stored time and each C-rate separately.

1 In the **Model Builder** window, click **Concentrations, All Species (tcd)**.

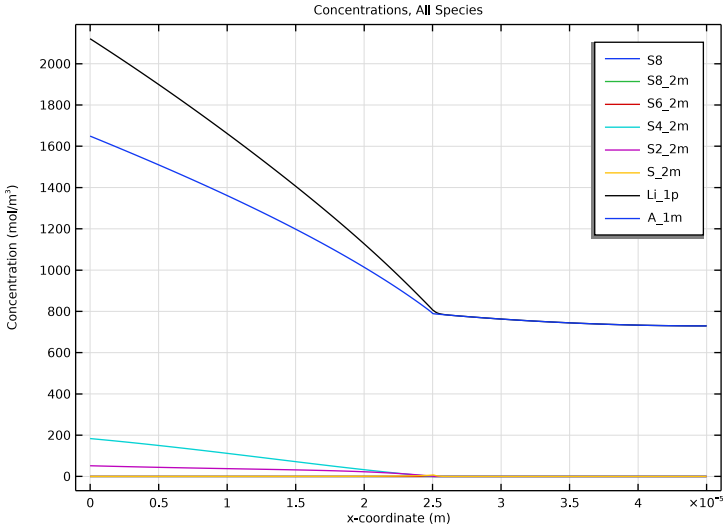
2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Time selection** list, choose **Last**.

4 From the **Parameter selection (C)** list, choose **From list**.

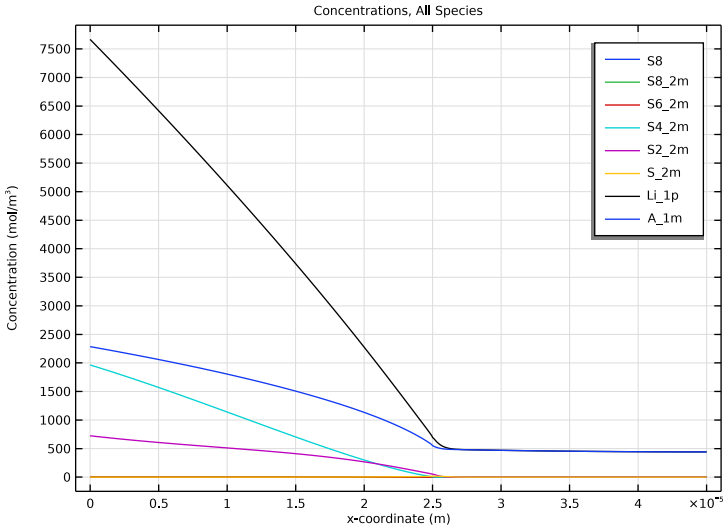
5 In the **Parameter values (C)** list box, select **0.2**.

6 In the **Concentrations, All Species (tcd)** toolbar, click **Plot**.



7 In the **Parameter values (C)** list box, select **1**.

8 In the **Concentrations, All Species (tcd)** toolbar, click **Plot**.



The remaining S-species in the electrolyte at 1C correspond to the reduced capacity (compared to 0.2C) seen in the cell voltage plot.

Precipitated Li2S(s)

Finally, proceed as follows to plot the volume fraction of the precipitated Li2S(s) in the electrode. This plot is a good indicator of how uniform the current distribution in the electrode is:

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Precipitated Li2S(s)` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Label**.

Line Graph 1

1 Right-click **Precipitated Li2S(s)** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **eps_Li2S_s - Volume fraction, Li2S(s) - 1**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `Li<sub>2</sub>S(s)`.

8 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Color table**.

Precipitated Li2S(s)

1 In the **Model Builder** window, click **Precipitated Li2S(s)**.

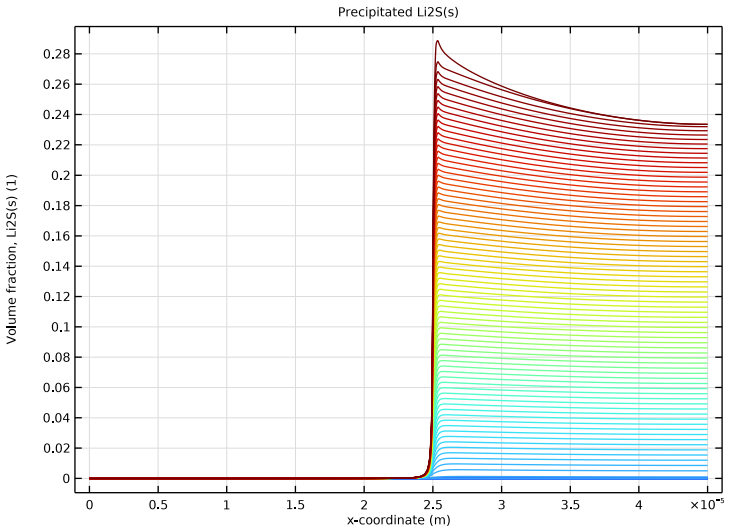
2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

4 From the **Parameter selection (C)** list, choose **From list**.

5 In the **Parameter values (C)** list box, select **0.2**.

6 In the **Precipitated Li2S(s)** toolbar, click **Plot**.



7 In the **Parameter values (C)** list box, select **1**.

8 In the **Precipitated Li2S(s)** toolbar, click **Plot**.